Modeling Drying / Hydration / Carbonation in thin mortars using CEMHYD3D

Franck VALLEE - *Guest Researcher*

CSTB / LAFARGE / RHODIA

Building and Fire Research Laboratory

June 2000

National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Background

- Although special mortars used as thin coats (adhesives, coatings, renders,…) are becoming more and more sophisticated and represent constantly increasing markets, little scientific knowledge is currently available on these kinds of materials.
- A recent PhD study enabled us to get experimental data on the development of the microstructure of these composites

Objectives of the project

- Model the evolution of the microstructure of Polymer / Cement Composites (PCC) induced by weathering
- Increase the knowledge of the aging mechanisms of these types of materials
- Use computer modeling to predict the durability of such materials

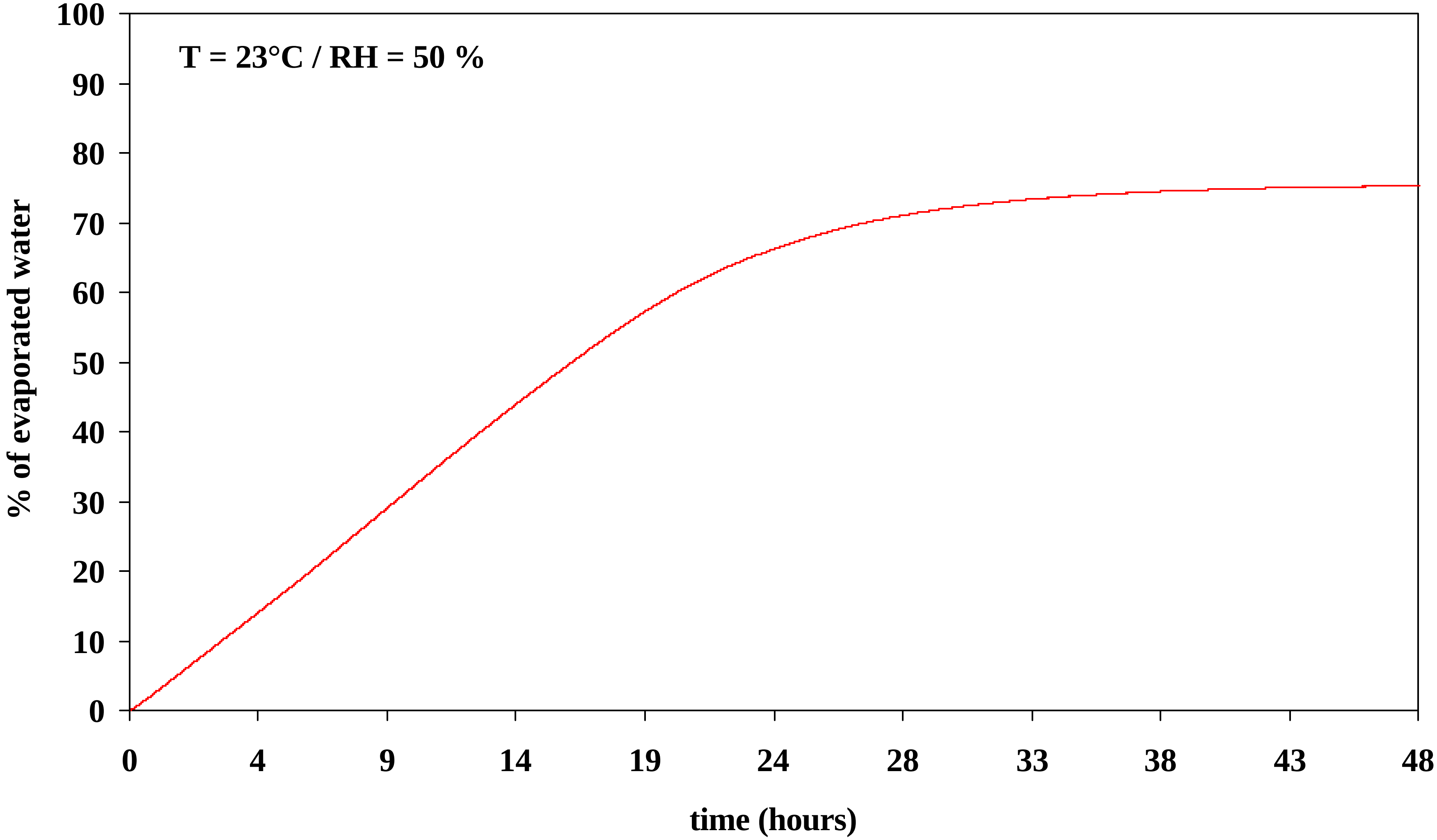
Steps :

- Modeling of the development of the microstructure of the mortars
- Modeling of the development of the microstructure of a thin layer cement paste specimen
- Observe the influence of the introduction of latex particles on the development of the inorganic matrix

Enhancements brought to the existing model

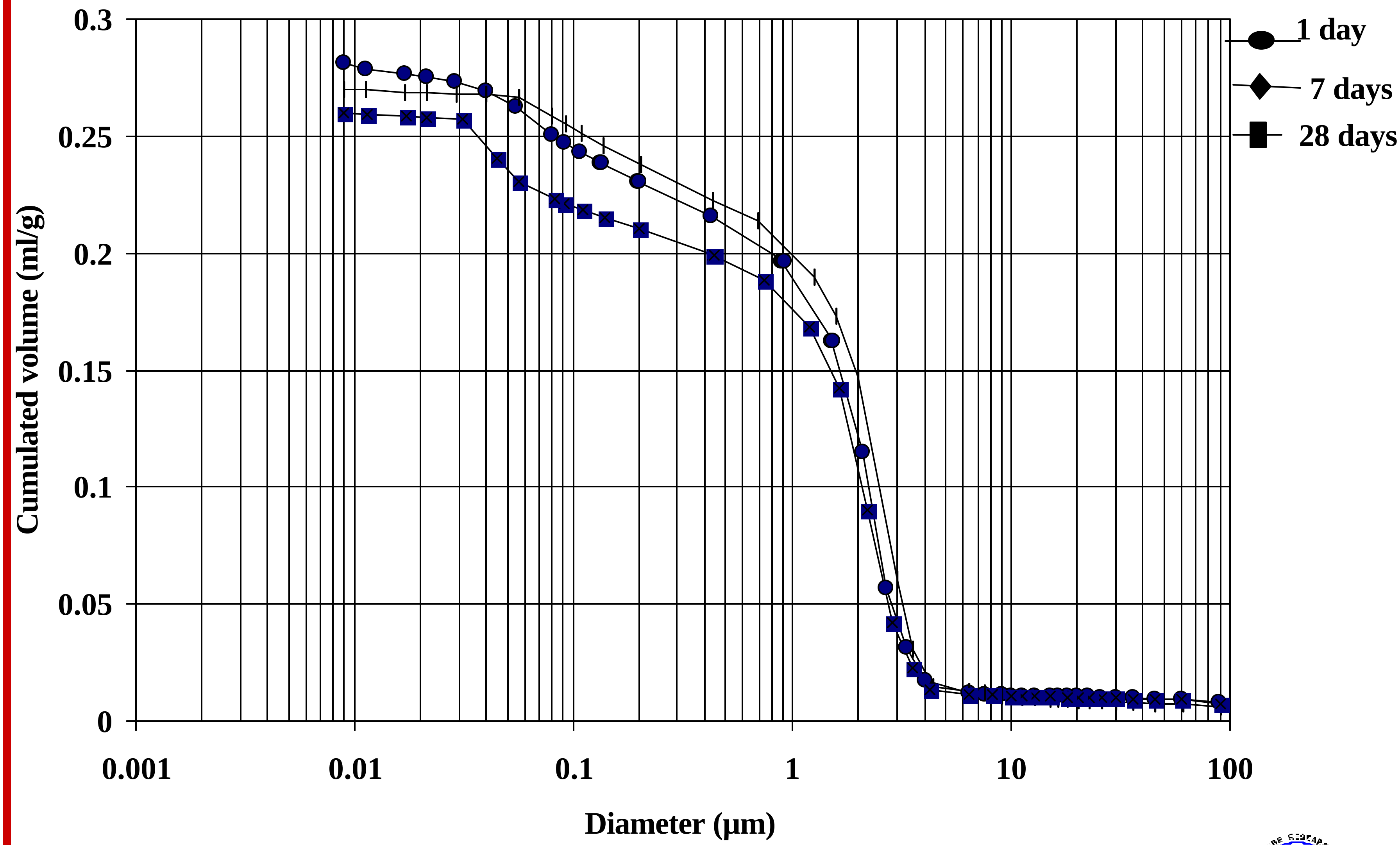
- Model dimensions (possibility to simulate structures of a few mm thick)
- Evaporation
- Carbonation

Water evaporation kinetics for a 3 mm thick cement paste (W/C = 0.6)



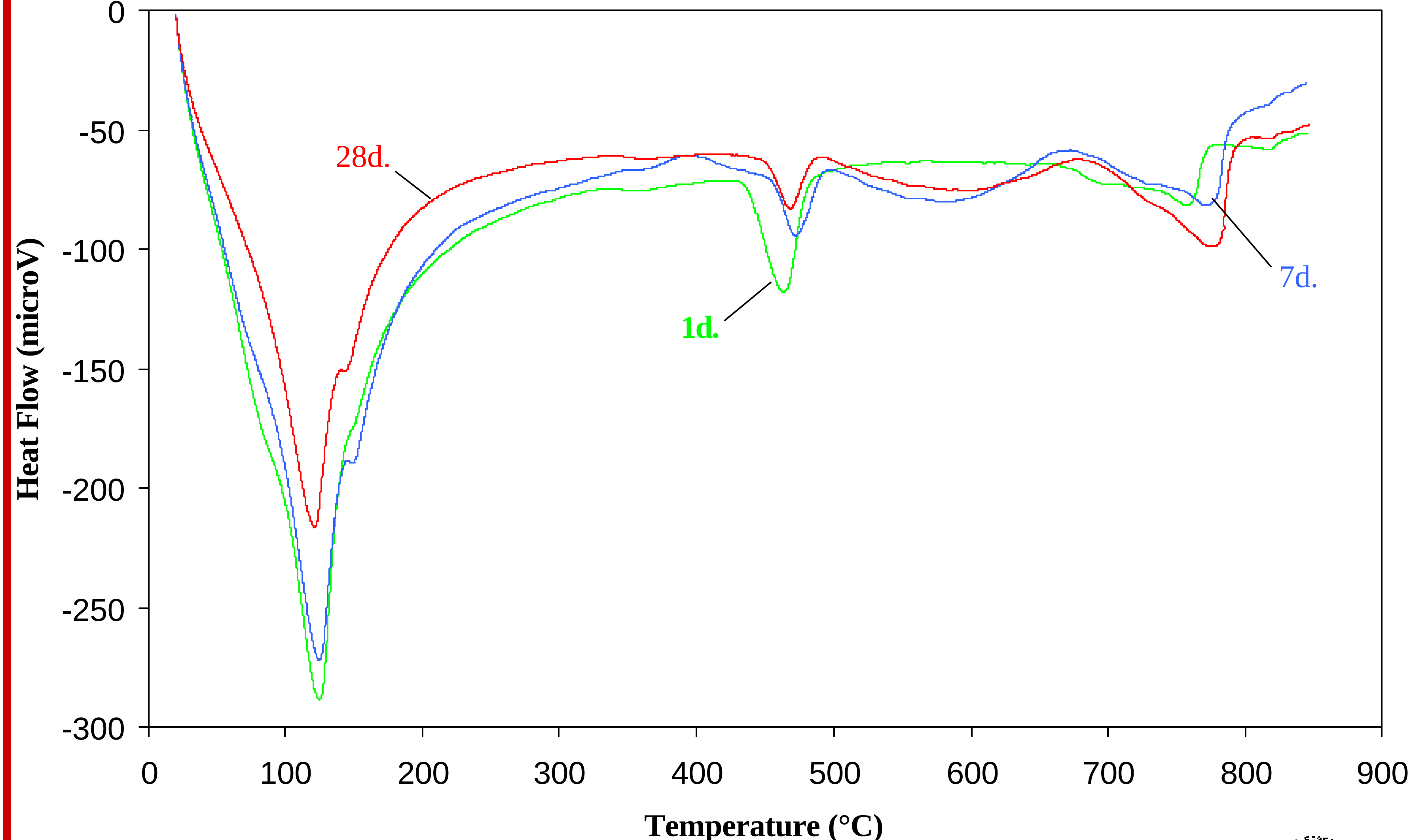
NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

MIP curves of a cement paste (w/c = 0.6) after 1, 7 and 28 days of cure



NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

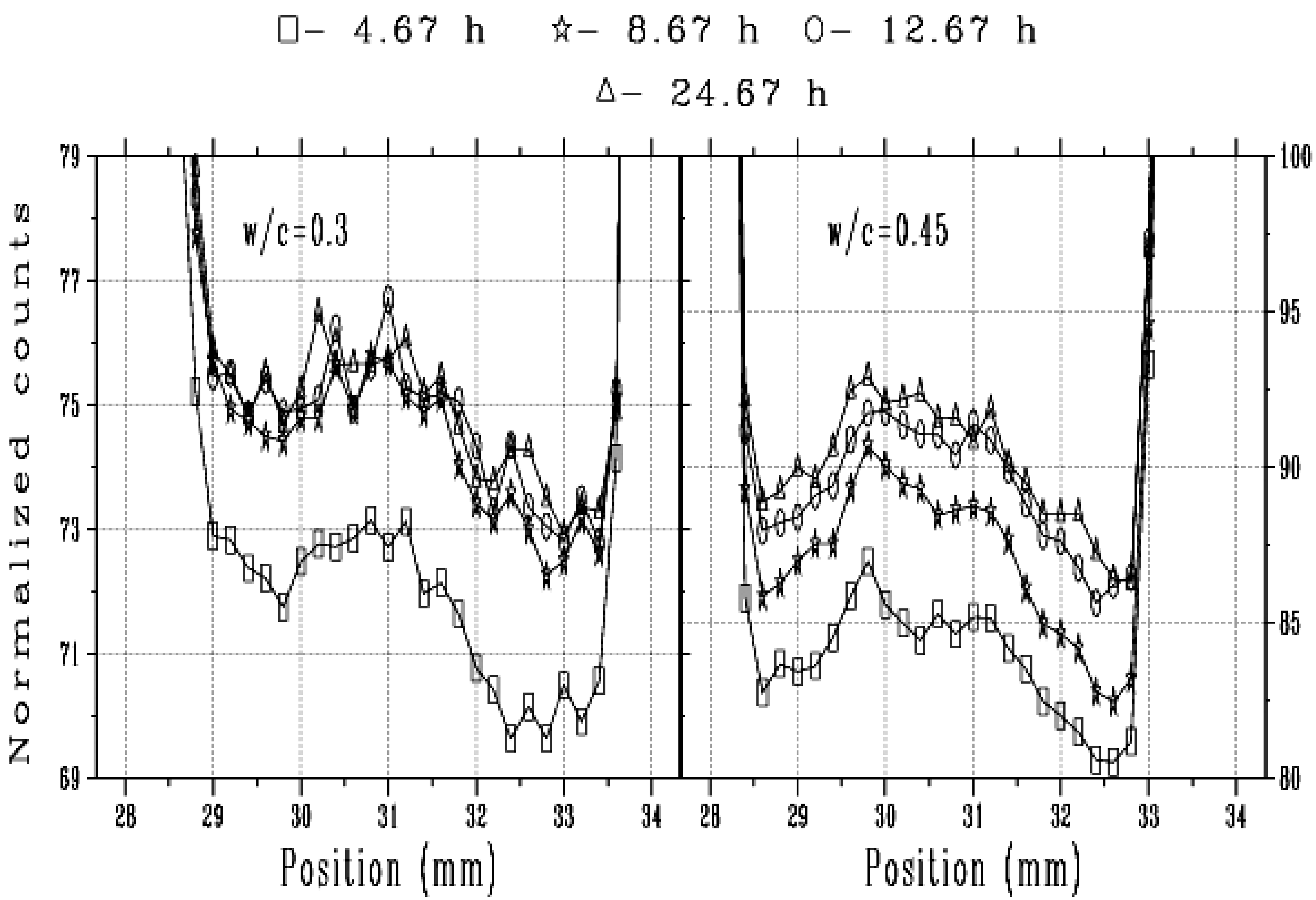
DTA curves of a cement paste (w/c = 0.6) at 1, 7 and 28 days of cure showing the phenomenon of carbonation



Evaporation algorithm

- Largest pore “spaces” within microstructure are emptied first at a user-specified drying rate (using a digitized sphere to assess local porosity)
- no sharp drying front (X-Ray observations)

Evaporation profiles
(X-Ray Absorption measurements)



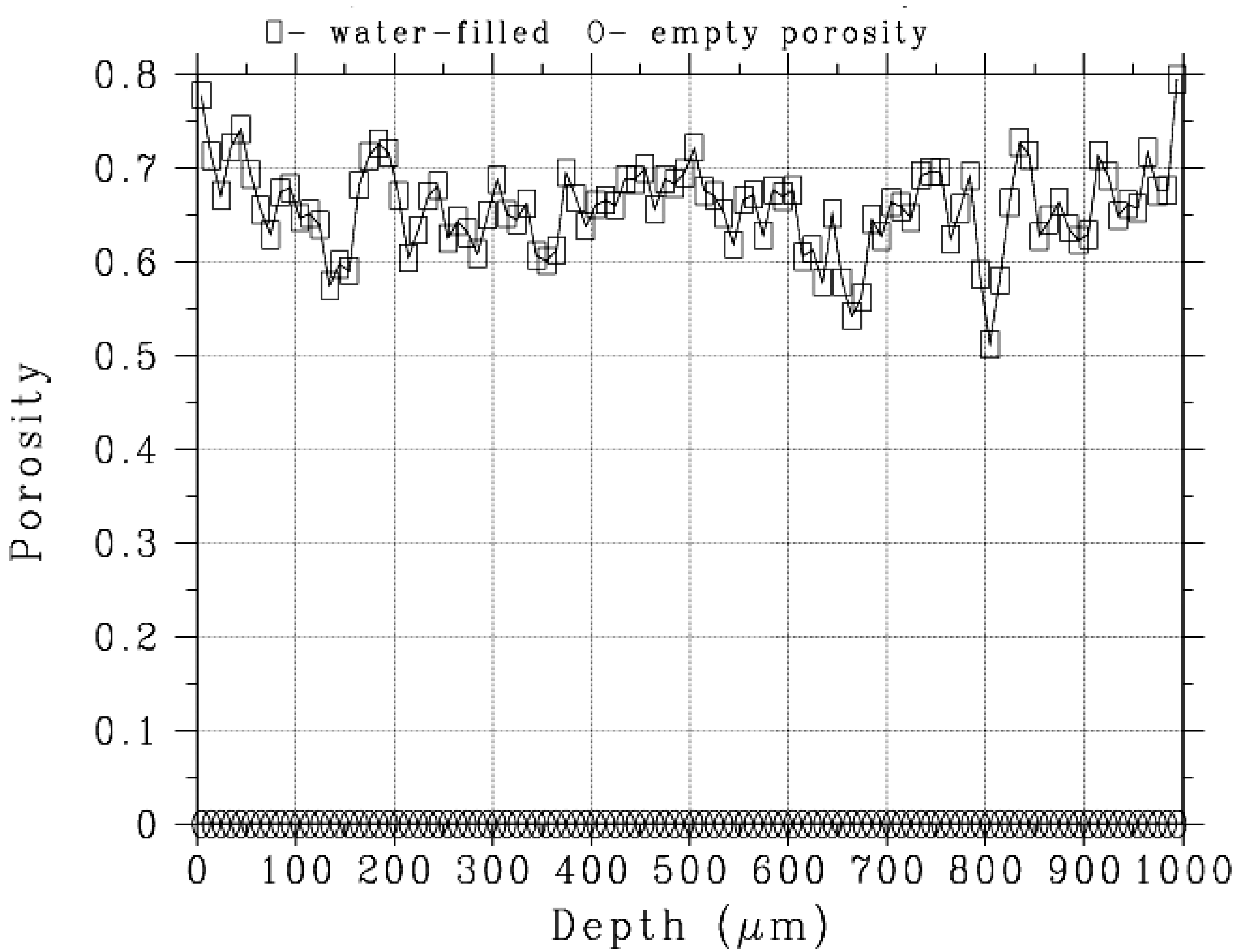
Carbonation algorithm

- CH converted to $CaCO_3$ with 11 % volumetric expansion at a user-specified rate
- sharp carbonation front (pixels of CH closest to exposed surface carbonate first)

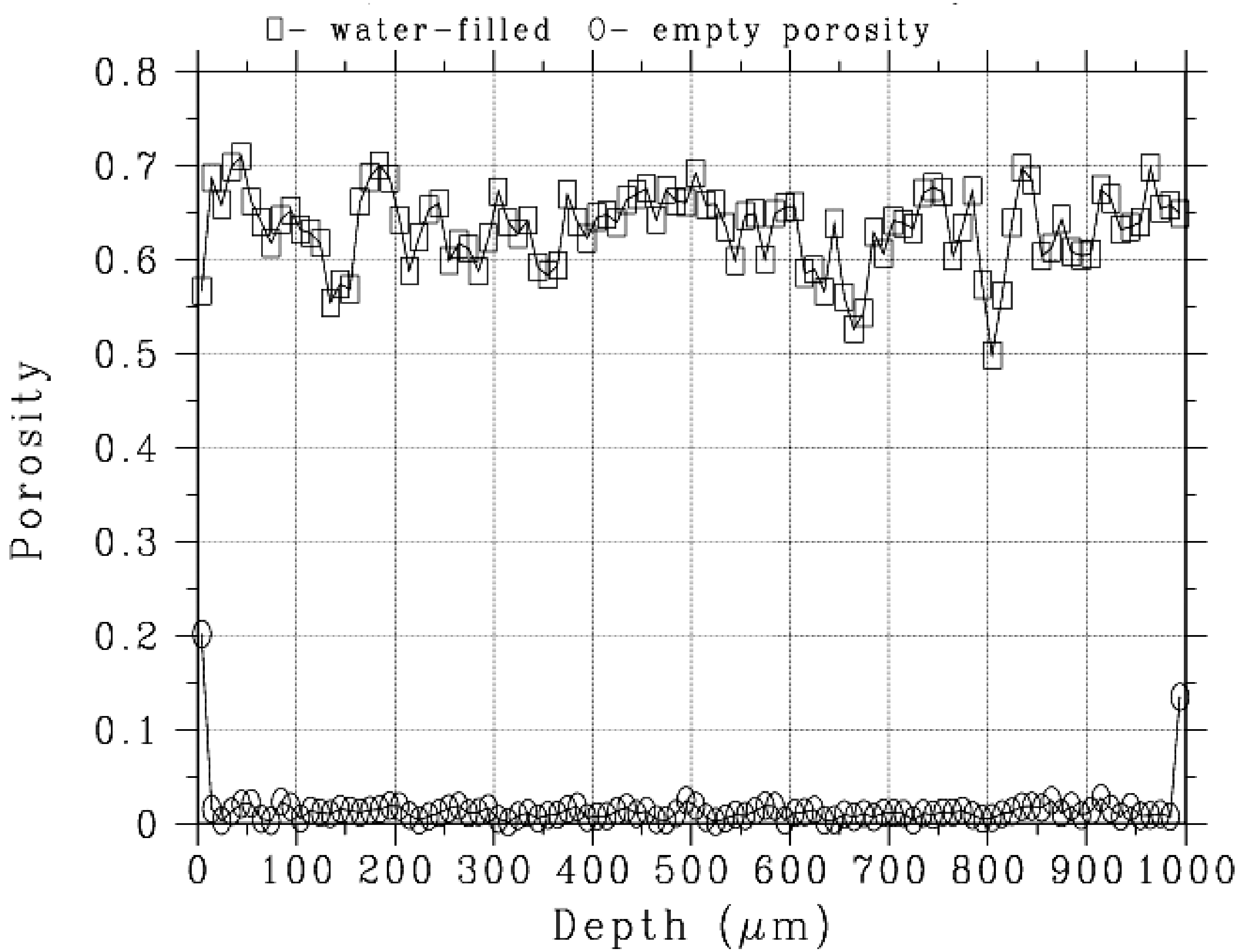
First results

- Structure 100x100x1000 microns
- Portland cement :
  - Blaine surface = 350 m^2 / kg
  - 58.6 % C_3S, 14.8 % C_2S, 10.6 % C_3A, 7.5 % C_4AF
- W / C = 0.6

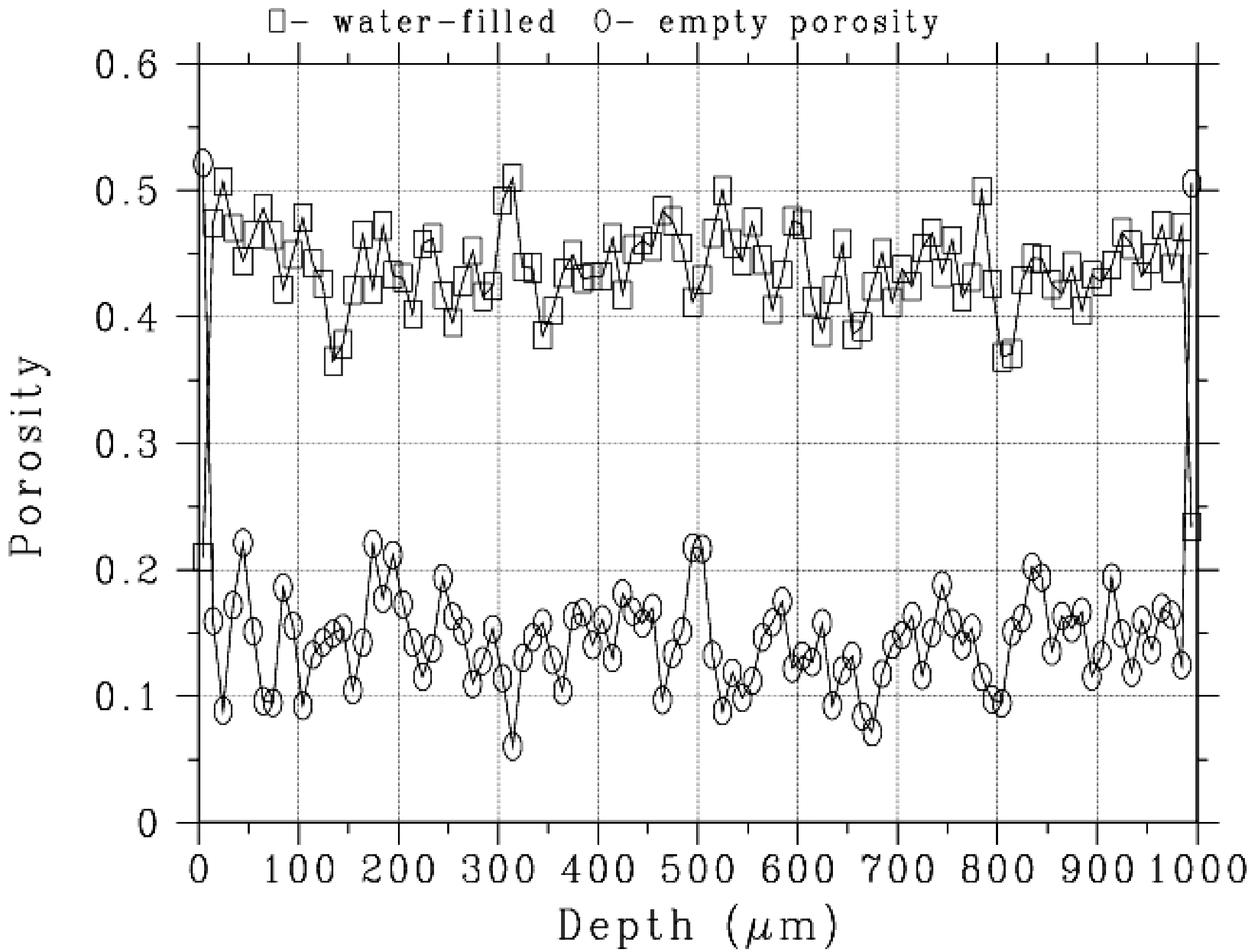
Porosity = f (depth) before hydration



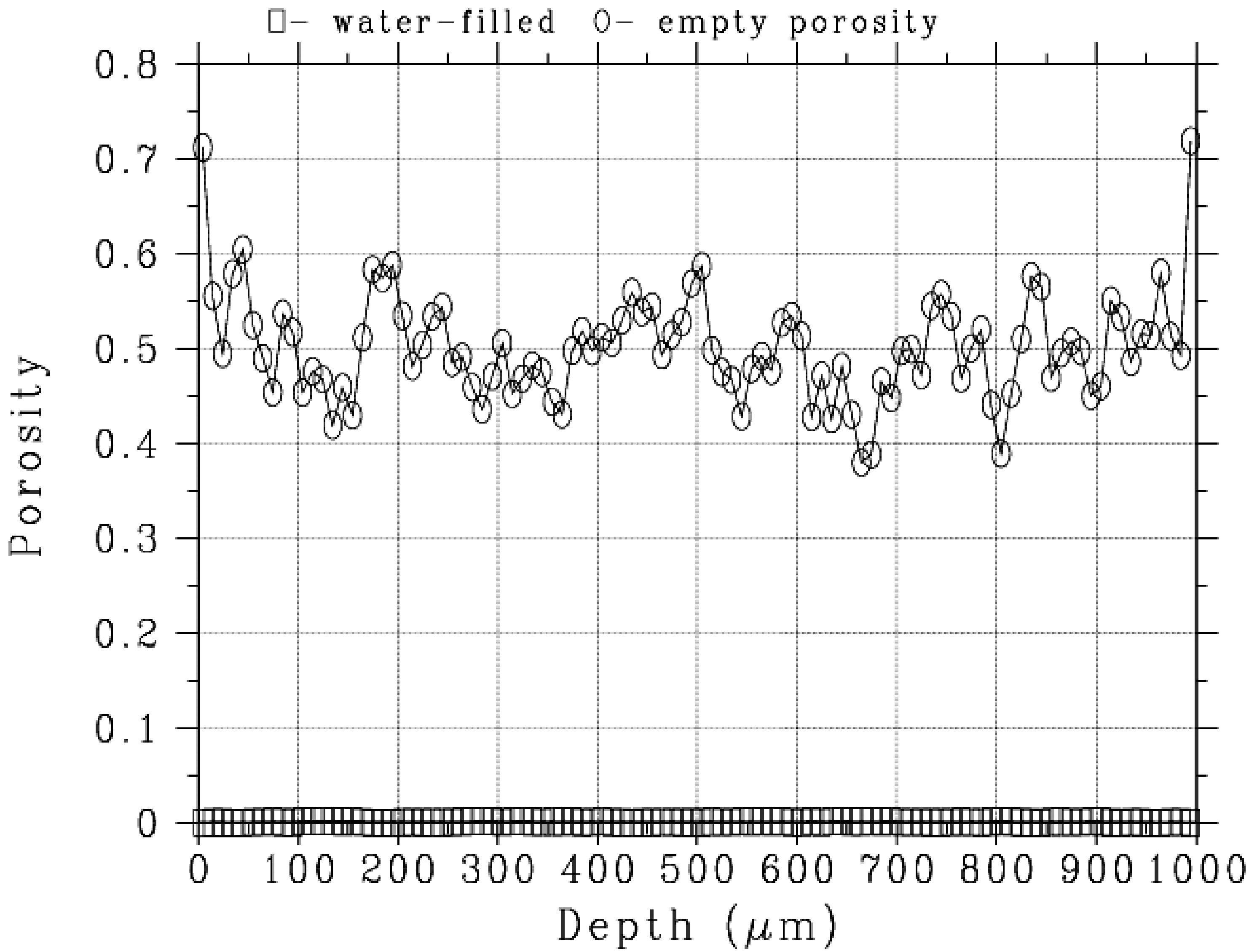
Porosity = f (depth) after 25 hydration cycles (0.7 h.)



Porosity = f (depth) after 75 hydration cycles (7 h.)

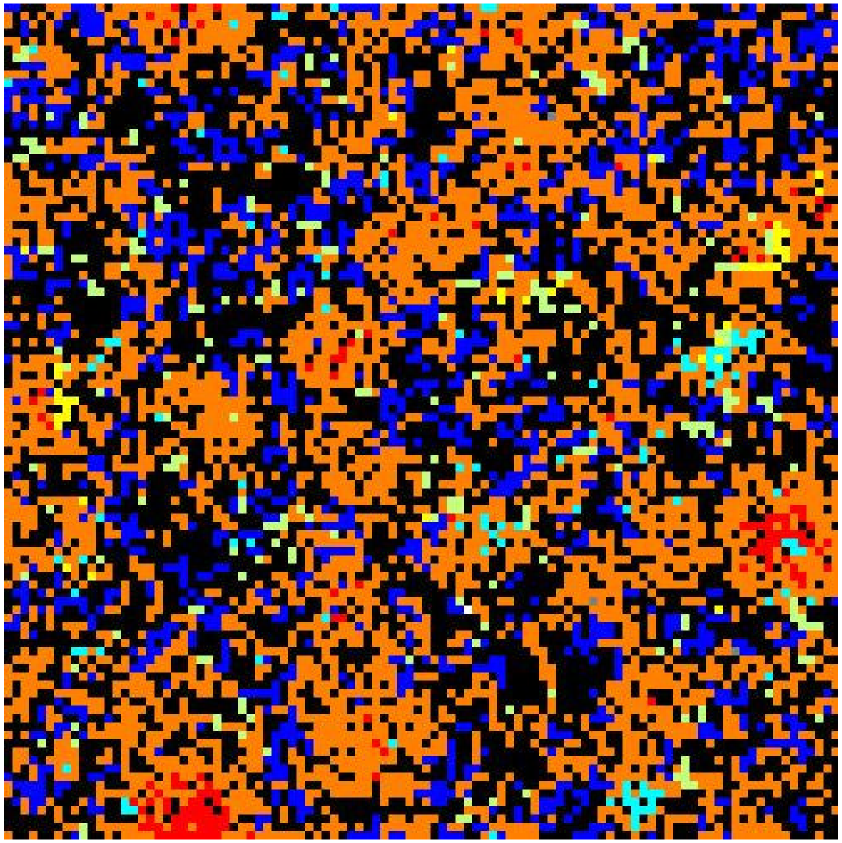


Porosity = f (depth) after 280 hydration cycles (90 h.)



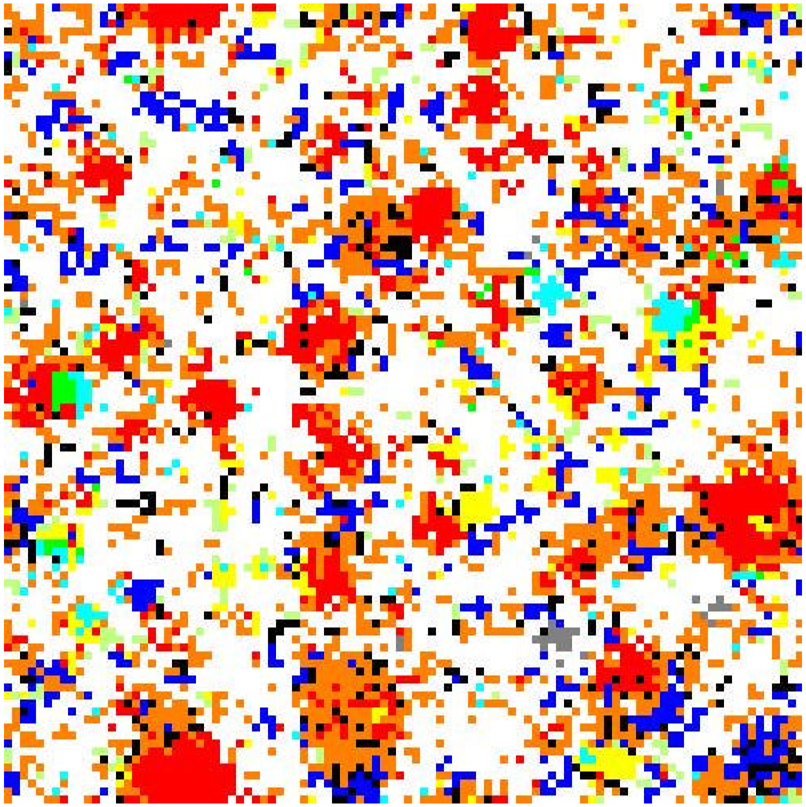
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Structure after 280 hydration cycles (90 h)
W / C = 0.6



red – C3S; orange - CSH; dark blue – CH; black – water filled porosity

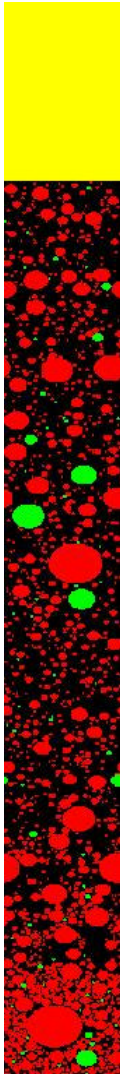
Structure after 280 hydration / evaporation cycles W / C = 0.6



red – C3S; orange - CSH;
dark blue – CH;
white – dried porosity

- **%ANH/PASTE = 38 % (40 % exp. SEM / IA)**
- **% POROSITY = 50 % (40 % exp. SEM / IA)**

Introduction of the settling



- %ANH/PASTE = 48 % (40 % exp.)
- % POROSITY = 44 % (40 % exp.)

Hydration with evaporation / settling / carbonation

	Exp. (SEM / IA)	Hydration + evaporation	Hydration + evaporation + settling	Hydration + evaporation + settling + carbonation
% ANH/PASTE	40	38	48	41
% POROSITY	40	50	44	37

Conclusions

- Very good correlation with the experimental data in terms of :
  - drying profiles
  - hydration level
  - porosity
- Model well adapted to simulate the development of the microstructure of a thin cement paste

Perspectives

- Simulate the aging of the pure cement paste
- Introduce latex particles in the system and observe the influence on the development of the inorganic matrix
- Simulate the aging of the composite and observe the influence on the evolution of the microstructure